

# Issues of Transparency, Testing and Validation in the Development and Application of Simulation Models

David J. Murray-Smith

University of Glasgow, School of Engineering, Rankine Building, Glasgow G12 8QQ, Scotland, United Kingdom;  
*David.Murray-Smith@Glasgow.ac.uk*

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**Abstract.** The importance of verification, validation and documentation of simulation models is widely recognised, at least in principle. However, in practice, inadequate model management procedures can lead to insufficient information being available to allow a model to be applied with confidence or for it to be re-used without difficulty and much additional effort. The ease with which a model can be understood by someone not involved in its development depends on the transparency of the model development process. This paper reviews ideas associated with transparency and model management. It also includes discussion of some related issues that are believed to be particularly important, such as identifiability and experimental design for model validation. Some recent developments in engineering applications and in physiological and health-care modelling are discussed, along with the responsibilities of the academic community in giving more emphasis to simulation model testing and transparency.

## Introduction

The testing, validation and detailed documentation of simulation models are all important issues in every field in which modelling and simulation techniques are used. It is also well-established that the development of simulation models involves an iterative process and that model testing is inseparable from all other aspects of model development. One very important milestone was the production in 1979 of the ground-breaking recommendations of the SCS Technical Committee on Model Credibility [1].

This provided a useful set of conventions and definitions for use in discussing the development of models and the main message about the importance of model testing and the iterative nature of modelling and simulation processes has since been emphasised repeatedly by many others, such as Sargent (e.g. [2]), Ören (e.g. [3]), Balci (e.g. [4]) and Brade (e.g. [5]).

Transparency in simulation model development is another closely-related issue and is concerned with the ease with which a model, its associated simulation software and testing procedures, can be understood by someone not involved in its development. This relates to questions of model management in general and to documentation in particular.

In the context of engineering applications, a simulation model that is used in the design of a new product may well have a continuing and significant role throughout the complete life-cycle of that product. The continuing value of a model will depend on how that model is managed from the outset, including the testing strategy, verification and validation processes, and the availability of useful information about all aspects of the model and its development [6].

In all application areas the increasing use of object-oriented software, the integration of simulation tools with other forms of specialist software, the availability of libraries of sub-models and the development of generic simulation models intended for use in a number of different applications are typical of ways in which modelling and simulation methods have been changing in recent years [6-8]. These changes of approach should have been accompanied by determined efforts to ensure transparency within the development process, through careful and systematic documentation, together with more rigorous procedures for testing, verification and validation.

However, there is clear evidence that these issues are still not being given appropriate attention by some model developers, users and also those involved in education [8-11]. Issues relating to model quality, such as the range of applicability of a given model, how the behaviour of a model can be compared with the behaviour of the corresponding real system, the precise experimental conditions used in comparing simulation results with real-world data and availability of documentation are seldom emphasised in published material.

This situation is made worse by the fact that many published journal papers and reports dealing with modelling and simulation applications lack real transparency in terms of the model and the simulation methodology being used and also include little about testing and validation results. How can students be expected to give more attention to these issues when they see that their lecturers and professors are still successfully publishing research papers in which scant attention appears to be given to these topics?

Another related issue is that, in some organisations, simulation modelling is often treated in a different way from other software development processes. Simulation models are often developed without the benefits of version control procedures that are a central feature of most software development environments. Should methods of approach to version control that have been used successfully in the software engineering field be applied to the development and management of simulation models?

There is also a clear need to consider why rigorous and systematic testing techniques that are currently available are not being applied more widely and why the documentation of models is too often superficial or non-existent. The consequent problems that follow on from these failings also need to be considered, together with consideration of the added short-term costs of adopting a more rigorous approach of this kind.

## 1 The Need for Good Model Management

As mentioned above, quality assurance mechanisms and model management procedures are often notably absent from the modelling and simulation processes within many organisations.

Whether models are developed from first principles, or reinstated from previous projects, or acquired from other organisations, appropriate strategies need to be in place to make sure that model quality issues are addressed properly and that all aspects of the modelling and simulation activities are managed in an appropriate fashion [5], [8-11]. This is important in all scientific, medical and decision making application areas as well as in engineering.

One important aspect of model management involves the establishment of a suitable plan for model verification, validation and approval and this needs to be started at the earliest stages of a model development project. Such a plan should lay down clear quantitative requirements for the validation for each element of the model, but with flexibility in terms of methods to be used. For example, preliminary assessment of a model on the basis of face validation may be followed by the application of a more quantitative approach as confidence increases. Where model libraries are being applied, validation information about sub-models should be brought together using the available documentation and reviewed in a critical fashion in the context of the intended application. The plan has to provide guidance for every aspect of model testing and has to be recognised as being quite different and distinct from the model specification. In addition, the plan for verification, validation and approval should outline the methods to be adopted and provide information about resources available from previous projects, such as fully-tested simulation models or sub-models.

Since the modelling process is iterative, the verification, validation and acceptance plan may itself have to be modified and fine-tuned as the work progresses. For example, as experience grows from analysis of test results from the real system, trade-offs may become necessary between the validation requirements and the quantity of additional validation data needed. Even if collection of test data from the real system is the responsibility of others, those involved in the model development process should be able to contribute to the planning of the model testing process since early experience with a simulation model may provide insight that influences the design of experiments. An example of this is the fact that understanding of parameter sensitivity issues built up during the model development process can contribute significantly to experimental design and to questions relating to model uncertainties.

On the other hand, the management system should ensure that, wherever possible, the assessment of test results and model results should involve blind comparisons. Initially, experimentalists should provide the simulation developers only with measured input data and other relevant information about test conditions. The simulation group would then use the input data provided by the experimentalists to make predictions of corresponding output variables. Experimental and simulation results could then be compared by members of both groups working together and conclusions reached about the adequacy, or otherwise of the model.

Documentation is another area where strict management procedures are important. Awareness of model limitations in the minds of users inevitably fades with time and accurate and easily accessible documentation is essential. This should deal with all aspects of the model including its purpose, assumptions and simplifications, details of verification and validation tests and an assessment of the range of conditions for which the final accepted model can be used. The documentation should also include information about the model variations developed during the project, together with reasons for accepting or rejecting each of these [8].

### 1.1 Model management practices

Reliable and easily-used methods for model version control are essential for large and complex models. This is particularly important when models are developed and maintained by a team rather than by an individual. Interactions between models of different types can also be an important feature of a project and it is important to ensure that no data transfer errors can occur between models. In addition, it is essential to ensure through an appropriate management system that whenever changes are made all of the relevant models are updated at the same time.

It has been suggested that model documentation should always be divided into two distinct sections (e.g. [8]). The first would involve non-technical documentation and would be accessible by all having some interest in the model and its applications. This section of the documentation would include an overview of the model in terms of its purpose, intended applications, variables, equations, parameters etc, together with a summary of the verification and validation procedures, detailed verification and validation results and resulting recommendations in terms of the range of conditions over

which the model could be used. The second section would provide all the additional information that would be required by someone wishing to make use of the model or to reconstruct the model and reproduce results that had been obtained previously. Splitting the documentation in this way means that aspects of a model regarded as being in some way confidential could be held back while still providing interested parties with a broad outline of the model and its capabilities.

The choice of software tools to assist in the management of models, simulation programs and the documentation depends on the computing environment being used. Details of the systems for keeping track of model versions, simulation programs, parameter values, validation data sets and results are also going to be different for different types of organisation. For example, in academic environments, large research groups may benefit from relatively rigid and centralised systems for model version control. On the other hand, an individual researcher working with one or two research students may find advantages in a simpler and less formal approach which just involves establishing a systematic way of keeping track of different model versions, of linking them to the appropriate data sets and to the corresponding simulation programs. Results of verification and validation tests must also be readily available and be easily linked to each model version. In large organisations the way in which this control can be achieved are clearly very different, especially when teams are geographically dispersed, when a more formal system of management becomes really important.

### 1.2 Benefits versus costs in model management

One ever-present issue that has to be considered in any organisation, whatever its size, concerns the costs of establishing systems of model management which involve comprehensive verification and validation procedures and large amounts of documentation. The recurrent expenses associated with such systems can be considerable. However, the costs resulting from failure to establish appropriate systems for the management of models can be much greater. In an engineering application, for example, the use of an inappropriate model for design purposes may lead to very large amounts of unplanned expenditure when re-design becomes necessary. The later in the design project that the problems are discovered the larger the costs of rectification.

Prototypes that fail to meet performance specifications inevitably lead to time-consuming and expensive changes to hardware and software. Similarly, in areas such as scientific research, the use of an inappropriate model can result in false conclusions and possibly incorrect decisions in terms of subsequent directions of research or policy recommendations.

Proper model management procedures, model transparency and documentation are also very important because knowledge about models which resides only in the heads of model developers is likely to be lost as soon as those individuals move on to new areas of responsibility or to a different organisation. Such a loss is clearly very wasteful. The academic world particularly weak in this respect because work carried out by graduate students at Master's degree and PhD level is recorded mainly through dissertations and these seldom include the level of detail about models that is necessary to build upon what has been achieved. Where modelling forms an important aspect of the work being reported, some separate archiving system should be required to supplement and support the information provided in the published thesis and this should be accessible by all who have access to the thesis.

One way of attempting to control the costs of model validation is through the establishment of a link between the verification, validation and acceptance plan and the more general requirements analysis document that details the purpose of the model, its accuracy requirements and defines the broad strategy for its development. That requirements analysis document can then provide the basis for a project plan which includes estimates of the human effort and can indicate how tasks involved in the model development process can be split between individuals. Establishment of a plan of this kind that places due emphasis on model validation should also allow confidence to be built up about the fitness of a model for its intended application while, at the same time, allowing the overall cost to be monitored continuously.

It is always difficult to obtain information about procedures for model management adopted elsewhere and this is especially true in commercial organisations. However, a number of studies have been carried out. One of these is an investigation by Foss et al [12] which relates to system modelling and simulation activities within the chemical industry. The modelling process receives close attention, including issues of verification, validation and documentation, using information from

16 experienced modellers and simulation specialists in organisations in several different countries. Suggested developments as a result of that investigation relate mainly to improvements in modelling technology and the use of advanced modelling tools. Foss et al also provide some useful insights about how modelling and simulation activities are carried out within the industry [12]. A second investigation focussed its attention on the helicopter manufacturing industry and involved responses to a questionnaire which sought views on the use of system identification and parameter estimation techniques for tasks such as the validation of physically-based flight mechanics models [13]. Eight companies from North America and Europe responded and the answers to the questions posed showed considerable interest in model validation and in the use of these specific techniques, while emphasising the need for physically-based interpretations at all times.

Cost predictions in terms of a model-based approach to engineering design also receives attention in a document by Pace [10] which discusses large projects in the aerospace and defence sector. A case is put forward for more sharing of information about the costs of modelling and simulation activities in order to allow the development of more reliable costing procedures. Another factor is that models can only be maintained properly if they are seen to be important, either in economic terms or in terms of their future potential. The difficulties and costs of maintaining models over the complete life-cycle of the system or product have to be considered explicitly and it appears that some engineering organisations and companies are establishing technology groups which are tasked with maintaining models, their software and documentation and translating these to new software environments as necessary.

## 2 The Testing of Simulation Models

There are two distinct and separate aspects to the testing of simulation models. One of these is termed 'validation'" and this is concerned with the process of establishing how well (or otherwise) the mathematical and logical description gives behaviour in the model that agrees with the observed behaviour of the system that it describes [1].

When a real system is available for testing and direct comparisons can be made of the time histories of key variables, the process can be carried out using a range of different quantitative methods and measures. Examples of methods that have been successfully applied in the past include graphical comparisons of various kinds, the use of methods based on system identification and parameter estimation, parameter distortion methods and evolutionary computing methods such as Genetic Programming (see e.g. [6], [8] for outlines of these different approaches). ‘Face’ validation methods, in which the model behaviour is assessed by someone who has expert knowledge of the real system but was not involved in the development of the model, provide a useful alternative (see e.g. [8]). A model can never be ‘valid’ for all applications and must be assessed in terms of its suitability for some specified use. Often a combination of quantitative and face validation approaches are used and subjective and objective evidence has to be combined in some way in establishing whether or not the model is fit for purpose. Acceptance of a model for its application requires statements of the range of conditions over which it can be used and the associated accuracy of model predictions

The second aspect of testing is termed ‘verification’ and relates to the process of establishing that a computer implementation of a model corresponds to the underlying mathematical and logical structure for that model [1]. This involves systematic checks of simulation code to ensure that no errors are present and also algorithmic checks to establish that appropriate computational methods have been applied [8]. This is a simpler process than validation and it has been suggested that formal methods (and especially ‘lightweight’ formal methods) could be used [14].

Both aspects of the model testing process are vitally important and must be considered in a systematic way in any application of modelling and simulation techniques. In essence, validation is concerned with the question ‘Is this the right model to describe the given system?’, while verification deals essentially with the question ‘Is the software implementation of the simulation correct?’. Each time a model and the associated simulation are changed in any way the procedures of verification and validation must be repeated and the whole procedure of model formulation, model testing and model updating must be regarded as iterative process which may have to be repeated many times during the life of a simulation model.

Although, as mentioned above, there are many different approaches to model validation there is one overriding aspect of testing that is relevant whatever method is adopted. This relates to questions of experimental design. In many engineering applications (and also in dealing with many physiological and biomedical modelling applications) testing includes the use of input signals to perturb the system. This is of fundamental importance because the choice of test input signal has a direct bearing on the amount of information available about the system under investigation. It thus also has an important influence on the effectiveness of tests carried out for the purposes of validating a model.

### 3 Issues of Identifiability and Test Input Design

Dynamic responses measured from experiments involving the application of test inputs can provide a great deal of information that is not available from the analysis of steady-state conditions or from responses resulting from some imposed set of initial conditions. Experiments involving test input signals also provide a basis for many well-established techniques of system identification. This is an inverse modelling procedure in which the structure and parameters of a model are estimated from sets of measured input-output data from the real system. Such techniques may be important in the development of physically-based simulation models if significant uncertainties exist in terms of the model structure or parameter values. Note that this ‘model identification’ type of inverse problem has to be distinguished from the ‘causation’ type of inverse problem where, for a given model, one seeks to find inputs that produce a specified response [15]. This causation type of approach also has relevance for model validation, as discussed elsewhere (e.g. [8]).

One very important concept that is closely linked to parameter estimation and model testing is model ‘identifiability’. There are two types of identifiability problem and these can be classified as:

- a) ‘global’, ‘structural’, ‘deterministic’ or ‘a priori’ identifiability
- and b) ‘pathological’, ‘numerical’, ‘practical’ or ‘a posteriori’ identifiability.

As the names suggest, the first type of identifiability problem arises because of the structure of the model.

Such issues arise when, for example, a model has too many parameters to allow all of them to be found independently from any identification experiment involving any combination of test inputs. Identifiability of this kind is the minimum condition necessary to obtain estimates of all model parameters. Thus, if a model is found to be structurally unidentifiable certain parameters cannot be estimated independently of others and this has important implications for model validation since sets of independent values cannot be assigned to those parameters. The second type of identifiability problem is encountered when a structurally identifiable model is being investigated using data sets that are too short in relation to the dynamic characteristics of the model or where measured response data sets are corrupted by significant measurement noise. Measured response data sets thus have to be long enough to capture the essential characteristics of the system if they are going to be useful for model validation and also have to be relatively noise free.

In the case of linear models, methods for the investigation of structural identifiability are well known and many relate to a transfer function type of approach proposed by Bellman and Åström [16], to methods based on Taylor series expansions or to a Markov parameter matrix approach [17]. In the case of nonlinear models two approaches are currently available. The first involves linearisation of the model about suitable operating points to reduce the nonlinear problem to a series of linear problems for which one of the linear approaches may be used. The second approach involves a Taylor series expansion of observations [17], although it is recognised that this is difficult to apply in the case of complex models.

Test inputs that are good for the purposes of system identification are those that excite the dominant modes of the system and also cover a range of amplitudes that are appropriate for characterising possible non-linear behaviour. Test inputs that are judged to be good for the purposes of system identification and parameter estimation are also generally good test inputs for the purposes of model validation. This fact is well-established but is often overlooked within the modelling and simulation community.

Specific techniques of test input design that have been found to be particularly useful in the context of model validation include those based on the D-optimal criterion (where equal emphasis is placed on all the relevant parameters) and the truncated D-optimal crite-

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rion (where a sub-set of the relevant model parameters is emphasised) [18]. The use of these test-input design techniques within simulation model validation, together with discussion on the use of frequency-domain measures (such as spectral energy and coherence functions) in comparing the effectiveness of different inputs is attracting renewed interest and details of these methods may be found elsewhere, along with relevant case studies (see e.g. [6], [8]).

## 4 Developments in Some Specific Application Areas

### 4.1 Engineering developments

It is very clear that in safety critical application areas, such as aircraft design, the automotive industry, railway systems, the nuclear industry and in many areas of defence, models are now subjected to a thorough process of development that involves version control, testing and documentation. Careful selection of test inputs for the purposes of model validation is also typical of work in these application areas. This, in many cases, is due partly to requirements imposed by external regulators and safety authorities.

In recent years the importance of using modelling techniques in large projects has become a central part of the philosophy of the US Defense Science Board (DSB) in the context of the DSB Model-Driven Architecture [19-20]. Closely associated with the ideas of a Model-Driven Architecture is the concept of a 'model as a specification' This was promoted very actively by Terry Ericson and his colleagues at the US Office of Naval Research, as part of a drive for major enhancements in the use of modelling and simulation techniques in the context of ship design, construction and operation (e.g. [21-23]).

The approaches used in other, less controlled and less safety-critical areas can sometimes be equally rigorous. However, there is still plenty of evidence that in many contexts simulation models are being developed and used in ways that lack extensive testing and involve documentation that is inadequate for anyone attempting to re-use a model. The documentation also often lacks transparency and may be inadequate for supporting and maintaining the system represented by the model over its complete lifecycle.

The justification for this rather haphazard approach to modelling and simulation activities is often that the more rigorous approach adopted in safety-critical application areas cannot be afforded and that the approach adopted is ‘what has always been done’.

Such negative views of the significance of model testing and documentation fail to take proper account of the costs that could possibly be saved in the development and management of new products through a more rigorous approach. Although such savings are difficult to quantify, it is interesting to note that in some areas of industry and science new approaches to computational models are becoming well-established.

In the Unkited Kingdom one important example of this is the decision that all major new building and infrastructure projects funded by central government from 2016 must adhere to Building Information Modelling (BIM) Level 2 requirements. Level 2 BIM provides a common single and coordinated source of structured information for consultants, contractors and all other parties engaged in a large and complex project [24]. It involves the use of computer-based models and associated databases for visualisation, information retrieval, documentation and life-time maintenance and support, and promotes consistency and transparency. It is already being used for the Crossrail project in London and is an essential feature of the planned HS2 high-speed rail construction project between London, Birmingham and cities further north. Although not concerned primarily with dynamic system simulation, BIM can provide data for dynamic simulations, in terms, for example, of building energy simulations and optimisation.

Future developments lie with Level 3 BIM and will require full collaboration between all parties involved in a project through the use of a single, shared project model held in a central repository. Everyone involved will then be able to access and modify that same model, and the benefit is that it eliminates risks associated with conflicting information. Industry concerns about commercial sensitivity and copyright issues are being resolved through robust documentation and software control procedures.

This requirement from the UK government is one aspect of a plan for reducing waste in the construction industry by 20%. It is believed that discrepancies, mistakes and inefficiencies in the information supply chain are major contributors to this waste and that collaborative working can significantly reduce it. Further BIM developments (at Levels 4D, 5D and 6D) involve the use

of BIM data to analyse time, for purposes of cost management and for facilities management.

It is interesting to note that BIM Level 3 has features that can be linked to the concepts of a ‘model as a specification’. The central and closely managed computer-based model of BIM Level 3 should provide a common reference point for all engaged in a project.

#### 4.2 Some developments in the modelling of physiological and health-care systems

Just as in engineering applications, the development of models of complex physiological systems needs to be made transparent to users. A systematic and properly managed approach is of great importance for the specification of a model, for development of model equations (including the choice of variables, parameters, model boundaries, assumptions and simplifications), for verification, for validation and for documentation. One interesting example from the biological sciences is the Human Physiome Project of the International Union of Physiological Sciences [25]. This is an initiative which is concerned with establishing a central repository of databases of experimentally-derived information and related computational models. The term ‘Physiome’ comes from ‘physio’ meaning ‘life’ and ‘-ome’ which means ‘as a whole’. The project aims to bring together, within one self-consistent framework, all the experimental and modelling elements of current physiological research. Contributors to the Human Physiome Project are from all parts of the world and simulation programs accepted for publication through this project may be downloaded and used by others. It is important to note that, within the Physiome Project, the word ‘model’ can be used to describe anything from a schematic diagram that suggests relationships between elements of a physiological system to a fully-tested and documented computer simulation model. Any model that is accepted is regarded as a ‘working hypothesis’ and has to form an internally self-consistent statement of the available information. What is especially interesting is that, through the processes of publication in the Physiome Project, the models and associated data sets provide an important stepping-stone to new experiments on the real system and thus to new models. Understanding of a given system should be enhanced in a step-by-step fashion through this type of collaborative procedure which involves an iterative process of modelling, simulation, testing and comparison.

One important feature of the Physiome Project is that all models have to pass through a ‘curation pipeline’ prior to being accepted and made available publicly. This procedure is similar to an independent review process for a conventional publication and is a form of ‘accreditation’. Within the curation procedure the submitted simulation model is tested to ensure that it is semantically sound and results obtained from it are consistent with the available published information about the corresponding real system.

In the health care systems modelling field one significant development in 2012 was the publication of seven papers prepared by the Good Research Practices in Modeling Task Force. This group was established in 2010 by the International Society for Pharmacoeconomics and Outcomes Research (ISPOR) and the Society for Medical Decision Making (SMDM). The Task Force produced a set of recommendations and seven articles were jointly published by both societies in their respective journals. A summary of the articles was presented as a plenary session at the ISPOR 16<sup>th</sup> Annual International Meeting in May 2011 and again at the SMDM 33<sup>rd</sup> Annual Meeting later that year and [26] provides an overview. Of the six other papers published by the Task Force members, the two most directly relevant to the theme of this paper focus on parameter estimation and uncertainties [27] and on ‘best practices’ in terms of model transparency and validation issues [28]. Many of the best practice recommendations are directly relevant to modelling and simulation in general and are not limited to applications involving health care. Most correspond to general issues of model management, testing and documentation discussed in this paper.

## 5 Discussion and Conclusions

Model management procedures should ensure that the model development process is reliable and robust. Good documentation standards should lead to high levels of transparency in the models created within such a management system.

Helpful insight in terms of good practice can be obtained from work on safety-critical and defence-related projects but issues of national or commercial secrecy limit transfer of knowledge from these fields into other areas of application. On the other hand, some very positive developments have also taken place recently in a number of areas of biomedical and healthcare modelling

and interesting recommendations have followed in terms of transparency and validation.

Recent developments in areas such as ship design and civil engineering also suggest that, with some external pressures initially, good modelling practice can produce significant benefits and potential cost savings in large projects. Current trends in those areas need to be considered to establish whether or not the ideas behind such developments could be transferred to other fields.

Education and training undoubtedly has an important influence. Many students encounter the ideas of mathematical modelling and computer simulation but relatively few graduates appear to be fully aware of the importance of testing their models. The emphasis in many courses is on the development of models from the underlying laws of physics, chemistry and other areas of science and then on the numerical methods for finding solutions. An examination of syllabus information from a wide range of universities suggests that, in many courses involving simulation, the topics of model testing, validation and documentation do not receive sufficient attention.

Another interesting point that relates to a number of scientific disciplines (e.g. the biological sciences) is that the convention in publication of experimental or computational results in a journal or conference proceedings is that a ‘methods’ section is traditionally included. The inclusion of the methods section is intended to provide enough information to allow readers to fully understand the techniques used to obtain the published results and, ideally, to allow readers to follow the processes used and thus repeat the results independently and be able to reproduce the published findings. Unfortunately, this is not a convention that is widely followed, at present, in most published work on modelling and simulation applications but has clear benefits in terms of establishing transparency and reproducibility.

Clearly, there are several areas in which there is scope for improvement in the processes of developing, implementing, documenting and applying simulation models within many organisations. It is clear that recent developments in some specific fields have led to interesting and helpful ideas and to recommendations in terms of best practices. Many of these ideas are transferable to other areas and are worthy of careful consideration by all engaged in modelling and simulation and especially by those involved in education.



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